



Piecewise Interpolants on Matrix Lie Groups

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Abstract—Here we consider a numerical procedure to interpolate on matrix Lie groups. By using the exponential map and its $(1, 1)$ diagonal Padé approximant, piecewise interpolants may be derived. The approach based on the Padé map has the advantage that the computation of exponentials and logarithms of matrices are reduced. We show that the updating technique proposed by Enright in [1] may be applied when a dense output is required. The application to the numerical solution of a system ODEs on matrix group and to a classical interpolation problem are reported. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords—Piecewise interpolants, Lie groups.

1. INTRODUCTION

In recent years, numerical analysts have shown a growing interest in numerical methods on Lie groups: for instance in the solution of ODEs whose solutions evolve on Lie groups, in finding the zeros of nonlinear equations or in the interpolation of elements of a Lie group (see [2–4]). Let \mathcal{G} be a Lie group and \mathfrak{g} its Lie algebra (see [5] for the definition of Lie group and of its Lie algebra). In this paper, we study methods to obtain a continuous interpolation on matrix Lie groups. In particular, we suppose that

$$Y_0, Y_1, \dots, Y_n$$

are the values that a continuous unknown real matrix function $Y : \mathbb{R} \rightarrow \mathcal{G}$ assumes on the set $\{t_0, t_1, \dots, t_n\}$. We wish to find a continuous matrix function $P : \mathbb{R} \rightarrow \mathcal{G}$ which belongs to the same matrix Lie group \mathcal{G} for all t and such that

$$P(t_i) = Y_i, \quad i = 0, 1, \dots, n.$$

Polynomial interpolation of matrices of a matrix Lie group is frequently undertaken in engineering applications (see [6]) or in the numerical solution of ODEs on matrix groups when a dense output is required (see [3]). From a computational point of view the main problem to be solved is that the interpolation must belong to the matrix Lie group considered. In fact the usual Lagrange interpolation does not guarantee $P(t)$ in \mathcal{G} for each t . In this paper, we concentrate our attention

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on interpolation in *quadratic groups* of matrices (see [7]). Let W be a nonsingular, symmetric or skew-symmetric $d \times d$ matrix. The *quadratic group* $\mathcal{H}(d, \mathbb{R})$ related to W , is given by the set of all nonsingular matrices $Y \in \mathbb{R}^{d \times d}$ such that $Y^T W Y = W$. The Lie algebra \mathfrak{h} associated to $\mathcal{H}(d, \mathbb{R})$ is the set of all $A \in \mathbb{R}^{d \times d}$ such that $A^T W + W A = 0$. If W is the identity matrix I_d of size d , we obtain the orthogonal group of the matrices of size d , $\mathcal{O}(d, \mathbb{R})$, with Lie algebra given by the set of skew-symmetric matrices

$$\mathfrak{o}(d, \mathbb{R}) = \{A \in \mathbb{R}^{d \times d} \mid A^T + A = 0\}.$$

If $W = J$, where

$$J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix},$$

we obtain the symplectic group $\mathcal{Sp}(2d, \mathbb{R})$ with Lie algebra given by the set of the Hamiltonian matrices $\mathfrak{sp}(2d, \mathbb{R}) = \{A \in \mathbb{R}^{2d \times 2d} \mid A^T J + J A = 0\}$. The Lorentz group $\mathcal{L}(d, \mathbb{R})$, with $d = p + m$, is the quadratic group of the diagonal matrix $W = \text{diag}(I_p, -I_m)$.

For solving interpolation problems on a matrix group, numerical procedures have been recently proposed (see [3,8]). Such methods are based on the transformation of the problem into an equivalent problem on the Lie algebra of the group (which is a finite dimensional vector space) where standard interpolation methods may be applied similarly to the procedure used to solve ordinary differential systems on Lie groups (see [9] for orthogonal systems and [10] for quadratic groups). The major computational difficulty with these methods is when a dense output is required: in this case exponentials of matrices at several points different from the grid points have to be evaluated. Here we will show that the use of piecewise continuous approximations allows us to apply an updating technique that reduces the cost of the method in the case of dense output. In particular, we will approximate $Y(t)$ by a matrix function of the following form:

$$P(t) = \mathcal{F}(\hat{A}(t)) Y_i, \quad t_i \leq t \leq t_{i+1}, \quad i = 0, \dots, n-1,$$

where $\hat{A}(t)$ on each subinterval $[t_i, t_{i+1}]$ is a continuous matrix function in the Lie algebra \mathfrak{h} of the group and \mathcal{F} is a map which transforms elements of \mathfrak{h} into elements of \mathcal{H} . It is well known that either the exponential map \exp or its diagonal (m, m) Padé approximant transforms elements of \mathfrak{h} into elements of \mathcal{H} . In particular we will employ the diagonal $(1, 1)$ Padé approximant of the exponential map, that is

$$\mathcal{R}(z) = \frac{1 + (1/2)z}{1 - (1/2)z}, \quad z \in \mathbb{C} - \{2\},$$

from which the following result holds.

THEOREM 1. (See [7].) *Let $\mathcal{H}(d, \mathbb{R})$ be the quadratic group of a matrix W and \mathfrak{h} its Lie algebra. All matrices Y of $\mathcal{H}(d, \mathbb{R})$ with $-1 \notin \sigma[Y]$ (where $\sigma[Y]$ is the spectra of Y) may be obtained by the Padé transform*

$$Y = \mathcal{R}(A) \tag{1}$$

with A matrix in \mathfrak{h} such that $2 \notin \sigma[A]$. Conversely, all matrices $A \in \mathfrak{h}$ with $2 \notin \sigma[A]$ may be obtained by the formulæ

$$A = \mathcal{R}^{-1}(Y),$$

with Y matrix in $\mathcal{H}(d, \mathbb{R})$ such that $-1 \notin \sigma[Y]$.

2. PIECEWISE INTERPOLANTS

For simplicity, we suppose that the interpolation points are equally spaced that is $t_{i+1} = t_i + h$, with $h > 0$ sufficiently small and $i = 0, 1, \dots, n-1$. We suppose that $Y(t)Y_i^{-1}$ is close to the matrix I for $t \in [t_i, t_i + h]$ and for any $i = 0, \dots, n-1$ and that $Y_i - Y_{i+1}$ is small enough so that $\|I - Y_{i+1}Y_i^{-1}\| < 1$ for any $i = 0, \dots, n-1$. In this section, we propose two piecewise interpolants based respectively on the exponential and Padé maps.

First, because of the features of the exponential map, we may assume the exact and interpolant function respectively in the following form:

$$Y(t) = \exp[A_i(t)]Y_i, \quad P(t) = \exp[\hat{A}_i(t)]Y_i, \quad t_i \leq t \leq t_i + h, \quad (2)$$

where $A_i(t)$ and $\hat{A}_i(t)$, on each subinterval $[t_i, t_i + h]$, are two continuous matrix functions in the Lie algebra of the group with $A_i(t_i) = \hat{A}_i(t_i) = 0$ for any $i = 0, \dots, n-1$. The previous form yields an interpolation matrix function $P(t)$ which belongs to $\mathcal{H}(d, \mathbb{R})$ for all t . Thus, by imposing the interpolation condition $P(t_i + h) = Y_{i+1}$, we can find the values of $\hat{A}_i(t)$ at the end point $t_i + h$ of $[t_i, t_i + h]$ that is

$$\hat{A}_{i,i+1} = \hat{A}_i(t_{i+1}) = \log(Y_{i+1}Y_i^{-1}), \quad i = 0, \dots, n-1, \quad (3)$$

where, from the previous assumption, $Y_{i+1}Y_i^{-1}$ is close to the identity matrix and $\log(Y_{i+1}Y_i^{-1})$ is well defined. Given $\hat{A}_i(t_i) = 0$ and $\hat{A}_i(t_{i+1})$, we may compute $\hat{A}_i(t)$ on $[t_i, t_i + h]$ by the linear interpolation that is we may consider $\hat{A}(t_i + \theta h) = \theta \hat{A}_{i,i+1}$, for $0 \leq \theta \leq 1$. Thus, the interpolant function, on each subinterval, is given by

$$P(t_i + \theta h) = \exp[\theta \hat{A}_{i,i+1}]Y_i, \quad 0 \leq \theta \leq 1. \quad (4)$$

It is easy to show that $P(t)$ is a second-order approximation of $Y(t)$.

THEOREM 2. *Let $\|\cdot\|$ be a matrix norm, then the following error estimate holds:*

$$\begin{aligned} \max_{t_0 \leq t \leq t_n} \|Y(t) - P(t)\| &\leq \frac{1}{8} h^2 \max_{0 \leq i \leq n-1} \left[\|Y_i\| \max_{0 \leq \theta \leq 1} \|A_i''(t_i + \theta h)\| \right. \\ &\quad \cdot \left. \max_{0 \leq \theta \leq 1} \left(\max_{0 \leq s \leq 1} \left\| \exp[(1-s)\hat{A}_i(t_i + \theta h)] \right\| \cdot \left\| \exp[sA_i(t_i + \theta h)] \right\| \right) \right]. \end{aligned}$$

PROOF. Suppose that t belongs to the time interval $[t_i, t_i + h]$, that is $t = t_i + \theta h$ for some $\theta \in [0, 1]$. Then from (2) it follows that

$$Y(t) - P(t) = \left(\exp[A_i(t)] - \exp[\hat{A}_i(t)] \right) Y_i, \quad t_i \leq t \leq t_i + h.$$

Since

$$\exp[A_i(t)] - \exp[\hat{A}_i(t)] = \int_0^1 \exp[(1-s)\hat{A}_i(t)] (A_i(t) - \hat{A}_i(t)) \exp[sA_i(t)] ds,$$

(see also [8]) and since $\hat{A}_i(t)$ is a second-order interpolant of $A_i(t)$ on $[t_i, t_i + h]$ we have

$$A_i(t) - \hat{A}_i(t) = \frac{1}{2} h^2 \theta(\theta - 1) A_i''(\mu_t), \quad \mu_t \in (t_i, t_i + h),$$

therefore, we may derive

$$\begin{aligned} \left\| \exp[A_i(t)] - \exp[\hat{A}_i(t)] \right\| &\leq \frac{1}{8} h^2 \max_{0 \leq \theta \leq 1} \|A_i''(t_i + \theta h)\| \\ &\quad \cdot \max_{0 \leq \theta \leq 1} \left(\max_{0 \leq s \leq 1} \left\| \exp[(1-s)\hat{A}_i(t_i + \theta h)] \right\| \cdot \left\| \exp[sA_i(t_i + \theta h)] \right\| \right) \end{aligned}$$

thus, the thesis follows. ■

If the orthogonal matrix Lie group and the 2-matrix norm are considered, the previous estimate becomes

$$\max_{t_0 \leq t \leq t_n} \|Y(t) - P(t)\| \leq \frac{1}{8} h^2 \max_{0 \leq i \leq n-1} \max_{0 \leq \theta \leq 1} \|A_i''(t_i + \theta h)\|.$$

When a dense output is required, then the interpolant $P(t_i + \theta h)$ must be computed at a certain number of points

$$0 < \theta_1, \theta_2, \dots, \theta_J < 1$$

that is

$$P(t_i + \theta_j h) = \exp[\theta_j \hat{A}_{i,i+1}] Y_i, \quad j = 1, \dots, J, \quad i = 0, \dots, n-1, \quad (5)$$

and the greater computational problem is now to compute $\exp[\theta_j \hat{A}_{i,i+1}]$ for each $j = 1, 2, \dots, J$. In practice, the exponential of a matrix is computed by means of (m, m) diagonal Padé approximants $\mathcal{R}_m(z)$, where $\mathcal{R}_m(z)$ is the rational function $\mathcal{P}_m(z)/\mathcal{P}_m(-z)$ with $\mathcal{P}_m(z)$ polynomial of high degree m . For instance the `expm` Matlab function computes $\exp(A)$ using the scaling and squaring algorithm based upon Padé approximation. Thus, from a computational point of view, (4) is replaced by

$$P(t_i + \theta h) = \mathcal{R}_m(\theta \hat{A}_{i,i+1}) Y_i, \quad 0 \leq \theta \leq 1,$$

which remains on the matrix quadratic group $\mathcal{H}(d, \mathbb{R})$, for each $0 \leq \theta \leq 1$, while (5) is replaced by

$$[\mathcal{P}_m(-\theta_j \hat{A}_{i,i+1})] P(t_i + \theta_j h) = \mathcal{P}_m(\theta_j \hat{A}_{i,i+1}) Y_i, \quad j = 1, \dots, J.$$

Thus, for a fixed i , the mathematical problem to be solved becomes the following: compute the set of linear matrix systems

$$[\mathcal{P}_m(-\theta_j A)] X = [\mathcal{P}_m(\theta_j A)] Y, \quad j = 1, \dots, J, \quad (6)$$

reducing the cost of the factorizations needed. A desirable feature is that the work made to factorize one matrix $\mathcal{P}_m(-\theta A)$ at a reference value of θ , for instance at θ_1 , may be used to compute the factorization of $\mathcal{P}_m(-\theta_j A)$ for $j = 2, \dots, J$. This problem may be seen as an updating technique and to solve it we can apply the updating procedure proposed by Enright in [1]. Recall this technique and for simplicity assume $m = 1$. In this case (6) becomes equivalent to

$$[A + \mu_j I] X = B_j, \quad j = 1, \dots, J,$$

where $\mu_j = -(2/\theta_j)$ and B_j is a known square matrix. The updating technique will provide a more efficient factorization of $[A + \mu_j I]$ for $j = 2, \dots, J$, given the following factorization of $A + \mu_1 I$:

$$A + \mu_1 I = L H L^{-1}, \quad (7)$$

where H is upper Hessenberg and L is unit lower triangular (that is the first step in the computation of eigenvalues of $A + \mu_1 I$). Then the decomposition of each of the remaining matrices would only require s adds since

$$A + \mu_j I = L [H + (\mu_j - \mu_1) I] L^{-1}, \quad j = 2, \dots, J.$$

Thus, if we perform the $L_j U_j$ factorization of the Hessenberg matrices $H + (\mu_j - \mu_1) I$, for $j = 1, \dots, J$, it follows that

$$A + \mu_j I = L [L_j U_j] L^{-1}, \quad j = 1, \dots, J.$$

A similar technique may be extended to the case of Padé approximation of high order m . Now we give the polynomial $\mathcal{P}_m(z)$ in terms of its roots, that is

$$\mathcal{P}_m(z) = \prod_{r=1}^m (z - \alpha_r)$$

thus,

$$\begin{aligned}\mathcal{P}_m(\theta_j A) &= \prod_{r=1}^m (\theta_j A - \alpha_r I) = (\theta_j)^m \prod_{r=1}^m (A - \mu_{rj} I), \\ \mathcal{P}_m(-\theta_j A) &= \prod_{r=1}^m (-\theta_j A - \alpha_r I) = (-\theta_j)^m \prod_{r=1}^m (A + \mu_{rj} I)\end{aligned}$$

where $\mu_{rj} = \alpha_r / \theta_j$. The systems in (6) become

$$\prod_{r=1}^m (A + \mu_{rj} I) X = (-1)^m \prod_{r=1}^m (A - \mu_{rj} I) Y, \quad j = 1, \dots, J,$$

thus, if $A + \mu_{11} I = LHL^{-1}$, we have

$$A + \mu_{rj} I = L[H + (\mu_{rj} - \mu_{11})I]L^{-1}, \quad r = 1, \dots, m, \quad j = 1, 2, \dots, J,$$

therefore,

$$\prod_{r=1}^m (A + \mu_{rj} I) = L \left[\prod_{r=1}^m [H + (\mu_{rj} - \mu_{11})I] \right] L^{-1} = L \left[\prod_{r=1}^m L_{rj} U_{rj} \right] L^{-1}, \quad j = 1, 2, \dots, J,$$

where $L_{rj} U_{rj}$ denotes the LU factorization of $[H + (\mu_{rj} - \mu_{11})I]$ for $r = 1, \dots, m$, and $j = 1, 2, \dots, J$.

To prevent a possible ill-conditioning of the systems arising in this approach it is possible to apply a pivoting technique in the computation of the factorization (7) so that the algorithm becomes stabler (see [1]).

In order to reduce the costs due to the computation of the logarithms and exponentials of matrices required in (3) and (5) we can employ the $(1, 1)$ Padé approximant of the exponential map. From Theorem 1, it follows that we may assume the exact and interpolant function, respectively, in the following form:

$$Y(t) = \mathcal{R}[A_i(t)]Y_i, \quad P(t) = \mathcal{R}[\hat{A}_i(t)]Y_i, \quad t_i \leq t \leq t_i + h, \quad (8)$$

where $\mathcal{R}(\cdot)$ is the $(1, 1)$ Padé map, while $A_i(t)$ and $\hat{A}_i(t)$, on each subinterval $[t_i, t_i + h]$, are two continuous matrix functions in the Lie algebra of the group with $A_i(t_i) = \hat{A}_i(t_i) = 0$ for any $i = 0, \dots, n-1$. We have to observe that when h is small, $A_i(t)$ and $\hat{A}_i(t)$ will have eigenvalues close to zero on $[t_i, t_i + h]$, thus, the Padé transforms of $A_i(t)$ and $\hat{A}_i(t)$ will be well defined.

From Theorem 1 it follows that the previous form yields an interpolation matrix function $P(t)$ which belong to $\mathcal{H}(d, \mathbb{R})$ for all t . Thus, by imposing the interpolation condition $P(t_i + h) = Y_{i+1}$, we find the values of $\hat{A}_i(t)$ at the end point $t_i + h$ of $[t_i, t_i + h]$ that is

$$\hat{A}_{i,i+1} = \mathcal{R}^{-1}[Y_{i+1}Y_i^{-1}], \quad i = 0, \dots, n-1, \quad (9)$$

where $\mathcal{R}^{-1}(\cdot)$ denotes the inverse map of $\mathcal{R}(\cdot)$ and $Y_{i+1}Y_i^{-1}$ is close to the identity matrix. Given $\hat{A}_{i,i+1}$ as in (9), we compute $\hat{A}_i(t)$ on $[t_i, t_i + h]$ by the linear interpolation that is we assume $\hat{A}(t_i + \theta h) = \theta \hat{A}_{i,i+1}$ for $0 \leq \theta \leq 1$. Thus, the interpolant function, on each subinterval, is given by

$$P(t_i + \theta h) = \mathcal{R}[\theta \hat{A}_{i,i+1}]Y_i, \quad 0 \leq \theta \leq 1.$$

THEOREM 3. Let $\|\cdot\|$ be a matrix norm, then the following error estimate holds:

$$\max_{t_0 \leq t \leq t_n} \|Y(t) - P(t)\| \leq \frac{1}{8} h^2 \max_{0 \leq i \leq n-1} \left[\|Y_i\| \max_{0 \leq \theta \leq 1} \|A_i''(t_i + \theta h)\| \right. \\ \left. \cdot \max_{0 \leq \theta \leq 1} \left(\left\| \left[I - \frac{1}{2} \hat{A}_i(t_i + \theta h) \right]^{-1} \right\| \cdot \left\| \left[I - \frac{1}{2} A_i(t_i + \theta h) \right]^{-1} \right\| \right) \right].$$

PROOF. Suppose that t belongs to the time interval $[t_i, t_i + h]$, that is $t = t_i + \theta h$ for some $\theta \in [0, 1]$. From (8) it follows that

$$Y(t) - P(t) = \left(\mathcal{R}[A_i(t)] - \mathcal{R}[\hat{A}_i(t)] \right) Y_i, \quad 0 \leq \theta \leq 1.$$

It is easy to see that

$$\mathcal{R}[A_i(t)] - \mathcal{R}[\hat{A}_i(t)] = \left[I - \frac{1}{2} A_i(t) \right]^{-1} (A_i(t) - \hat{A}_i(t)) \left[I - \frac{1}{2} \hat{A}_i(t) \right]^{-1}$$

from which the thesis follows. ■

If a dense output is required, then $P(t_i + \theta h)$ must be computed at a certain number of points. In particular at each i the following set of matrix linear systems must be solved:

$$[A_{i+1} + \mu_j I] P(t_i + \theta_j h) = -[A_{i+1} + \mu_j I] Y_i, \quad j = 1, \dots, J,$$

where $\mu_j = -2/\theta_j$, then the described updating technique may be applied.

It is obvious that the choice of the values $\theta_1, \theta_2, \dots, \theta_J$ may be different in each interval $[t_i, t_i + h]$ and the updating technique may be used likewise.

3. NUMERICAL TESTS

In this section, we describe the application of the piecewise interpolation technique to two particular problems: the solution of a system of ODEs and a classical interpolation problem and we compare the numerical results with two other methods that give a dense output. All the numerical results in this section have been obtained by Matlab codes implemented on a scalar computer Alpha 200 5/433 with 512 MB RAM.

EXAMPLE 1. We have considered the solution of the following system of ordinary differential equations:

$$Y'(t) = F(t, Y)Y(t)$$

with initial condition $Y(0)$ given by the identity matrix of order 4 and where

$$F(t, Y) = A - (YY^T - I)$$

with

$$A = \frac{1}{10} \begin{pmatrix} 0 & -1 & -1 & 3 \\ 1 & 0 & 2 & 1 \\ 1 & -2 & 0 & 1 \\ -3 & -1 & -1 & 0 \end{pmatrix}.$$

The theoretical solution is $Y(t) = \exp(tA)$ that is an orthogonal matrix for each $t \geq 0$, since A is skew-symmetric. We have first applied Runge-Kutta Munthe-Kaas method of order 3 with continuous weights, (see [3]), on the interval $[0, 3]$ taking step $h = 0.2$, then we have interpolated the numerical solution on the grid points using the (1, 1) Padé approximant as described in the previous section and comparing the continuous approximations given by both methods with the

Table 1.

Method	Flops
Continuous Munthe-Kaas	625822
Padé Approximant	408017

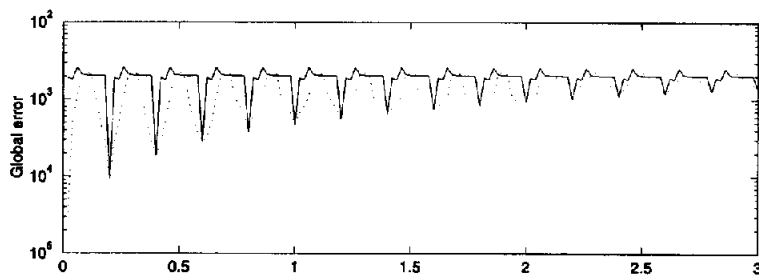


Figure 1.

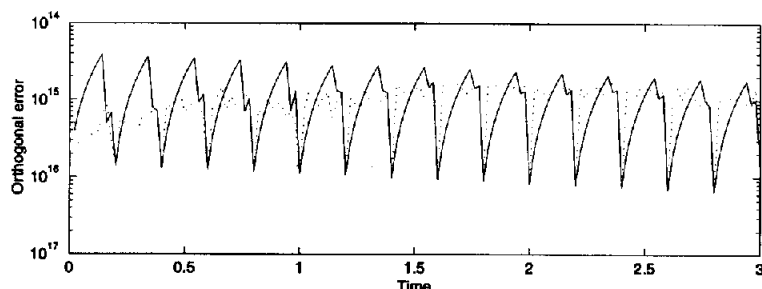


Figure 2.

theoretical solution. In Figure 1, we have plotted the global errors given by the continuous Munthe-Kaas method of order 3 (dotted line) and by the Padé approximation with the updating technique described in the previous section (solid line). In Figure 2, the orthogonal errors $\|I_4 - Y_k Y_k^T\|_F$ given by the same methods as in Figure 1 are shown. Both methods give similar errors but the Padé approximant do not require the computation of matrix exponential and then needs less flops (see Table 1).

EXAMPLE 2. In this case, we have considered a classical interpolation problem. We have a data set (t_i, Y_i) , $i = 0, 1, \dots, N$, such that

$$Y(t_i) = Y_i, \quad i = 0, 1, \dots, N,$$

where $Y(t)$ is a continuous matrix function. Hence, we have to compute an interpolating function $P(t)$ such that

$$P(t_i) = Y_i.$$

In this case, we have chosen the matrix function

$$Y(t) = (I - B(t))^{-1}(I + B(t)),$$

where

$$B(t) = \begin{pmatrix} 0 & t & 1 & 0 \\ -t & 0 & \cos(t) & \frac{1}{t^2 + 1} \\ -1 & -\cos(t) & 0 & -\frac{1}{t + 1} \\ 0 & -\frac{1}{t^2 + 1} & \frac{1}{t + 1} & 0 \end{pmatrix}$$

and we have computed the interpolating function on the interval $[0.5, 1]$ using first the method based on the Cayley transform (see [8]). In this case, the matrix function is approximated computing the Lagrange polynomial in the Lie algebra and setting this approximation in the Lie group by the Cayley transform. Then we have used the piecewise interpolant based on the $(1, 1)$ Padé transform with the updating technique. Finally, both approximations have been computed on a fine mesh. In the following table, we report the number of flops and the maximum error computed on the fine mesh. We note that the Padé method gives better results than the Cayley interpolant.

Table 2.

$N + 1$	Padé Interpolant		Cayley Interpolant	
	Flops	Error	Flops	Error
5	47392	2.0892	60021	2.9236
7	66759	1.0606	140183	1.4454
9	86465	$5.7620e - 1$	305769	$7.7821e - 1$
11	105119	$2.7774e - 1$	614603	$3.5783e - 1$
13	124157	$1.4914e - 1$	1140009	$1.5707e - 1$

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